PL-TR-96-2284

WAVENUMBER INTEGRATION SYNTHETIC SEISMOGRAM CALCULATIONS USING A PARALLEL VIRTUAL MACHINE

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July 1996

19970331 024

Scientific Report No. 1

DEPARTMENT OF ENERGY
Office of Non-Proliferation
and National Security
WASHINGTON, DC 20585

PHILLIPS LABORATORY
Directorate of Geophysics
AIR FORCE MATERIEL COMMAND
HANSCOM AFB, MA 01731-3010

SPONSORED BY
Department of Energy
Office of Non-Proliferation and National Security

MONITORED BY
Phillips Laboratory
CONTRACT No. F19628-95-C-0207

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
July 1996

3. REPORT TYPE AND DATES COVERED
Scientific Report No. 1

4. TITLE AND SUBTITLE
Wavenumber Integration Synthetic Seismogram Calculations Using a Parallel Virtual Machine

5. FUNDING NUMBERS
F19628-95-C-0207
PE 69120H
PR DENN TA GM WU AT

6. AUTHOR(S)
Keith L. McLaughlin and Boris Shkoller

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Maxwell Technologies - Federal Division
8888 Balboa Avenue, Bldg. 2
San Diego, CA 92123-1506

8. PERFORMING ORGANIZATION REPORT NUMBER
SSS-DTR-96-15561

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
Phillips Laboratory
29 Randolph Road
Hanscom AFB, MA 01731-3010
Contract Manager: Delaine Reiter/GPE

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
PL-TR-96-2284

11. SUPPLEMENTARY NOTES
This research was sponsored by the Department of Energy, Office of Non-Proliferation and National Security, Washington, DC 20585

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unilimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

The principal objectives of this work are to 1) provide more accurate, and efficient means to compute, store, and retrieve synthetic seismograms for reference layered Earth structures and 2) examine limitations of using layered Earth structures to model principal features of regional seismograms in the presence of lateral heterogeneity. This annual report describes work completed in the first year of this two year project and very briefly describes work to be carried out in the second year.

In the first year of this project a wavenumber integration program has been ported from a single processor application to a parallel processing environment using the Parallel Virtual Machine (PVM) software environment. This software allows the user to harness a network of UNIX workstations to perform calculations in parallel. A beta test version of the program is available upon request. Near linear speed-up over a single processor has been realized with a heterogeneous network tested over both wide and local area networks. Seismologists interested in serving as beta testers should contact Keith McLaughlin (*scatter@maxwell.com*).

14. SUBJECT TERMS
parallel processing — PVM
synthetic seismograms

15. NUMBER OF PAGES
28

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	SAR

Table of Contents

List of Illustrations

Figure **Page**

Summary

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In the first year of this project, a wavenumber integration program has been ported from a single processor application to a parallel processing environment using the Parallel Virtual Machine (PVM) software environment. This software allows the user to harness a network of UNIX workstations to perform calculations in parallel. A beta test version of the program is available upon request. Near linear speed-up over a single processor has been realized with a heterogeneous network tested over both wide and local area networks. Seismologists interested in serving as beta testers should contact Keith McLaughlin (*scatter@maxwell.com*).

Plans for the second year of the project include 1) improvements and bug fixes for the wavenumber integration program, 2) release of an X-windows graphical user interface, 3) generalizing frequency dependence of attenuation, Q(f), for the wavenumber integration program, 4) computation and compilation of synthetic seismograms for a library of layered Earth crustal structures, 5) comparison of layered crustal structures with 3D finite difference synthetics of layered crustal structures with random heterogeneity.

What is PVM?

All parallel computer algorithms are composed of modules which are executed on multiple processors, messages that must be sent between these modules, and strategies for coordinating the modules and processors to work in parallel. The modules are typically distributed over a set of processors that are connected in some sort of communications network. Much of the programming work to develop a parallel algorithm is focused on passing messages between these modules and synchronizing their work. Commercially available massively parallel processors (MPP) provide custom compilers and libraries to facilitate this kind of programming. However, most research institutions already have the makings of a parallel machine; they typically have several workstations connected in a local area network. The aggregate computing power of their workstations often exceeds the CPU power that might be available at a supercomputer center. Furthermore, these machines are often idle much of the day or night.

Parallel Virtual Machine (PVM) is a public domain software system for turning a network of computers into a virtual parallel computer. The software supports heterogeneous networks including nearly all UNIX workstations and many parallel and single processor supercomputers. Beta versions are available at time of this writing for LINUX, MS-Windows, and MS-NT PC based operating systems. The software is based on widely used TCP/IP message passing protocols and therefore functions over a wide variety of local area networks (LAN) and wide area networks (WAN). The user interface libraries are both *FORTRAN* (F77 and F90) and C callable from a user's program. PVM frees the user from the arcane details of TCP/IP message passing between programs (processes) by providing a high level C or *FORTRAN* user interface and providing buffering and routing daemons for to the TCP/IP packets on the user's computer. This is done by running *daemon* process on each processor that serve as a relay posts for all messages passed between the user's programs running on each processor. PVM may be obtained by anonymous ftp over the Internet from Oak Ridge National Lab and University of Tennessee by referencing the universal resource locator (URL) *http://www.epm.ornl.gov/pvm/pvm_home.html* with any web browser. Installation of PVM 3.3.11.requires an ANSI C compiler and can be accomplished in less than an hour.

Wavenumber Integration Synthesis -"The Perfect Parallel Algorithm"

Wavenumber integration calculations (Apsel and Luco, 1983) are computationally bound by the time it takes to compute the complex response between a source and a receiver for a given frequency. Wavenumber integration is also the "perfect parallel algorithm" because computation of one frequency 1) is independent of all other frequencies, 2) requires only a few input values, 3) results in only a few output values, and 4) there are many frequencies to compute. These programs are well suited to a m*aster - slave architecture*. The master program performs all file input/output and organizes the work of the many identical slave programs running on multiple processors in the network. We treat each slave program like a function call for each complex Green's function response at a fixed frequency and fixed source and fixed receiver. Figure 1 illustrates the concept behind the use

of the *master - slave* modules on a virtual parallel machine using PVM. The master program sends messages to the slave programs telling them which frequencies to compute and then waits for the results to return from the slaves in the form of messages. When the slave programs are not computing the response at a specific frequency, they are waiting for instructions from the slave program. The slave programs return the numerical results as well as timing information that is useful in load balancing the calculation.

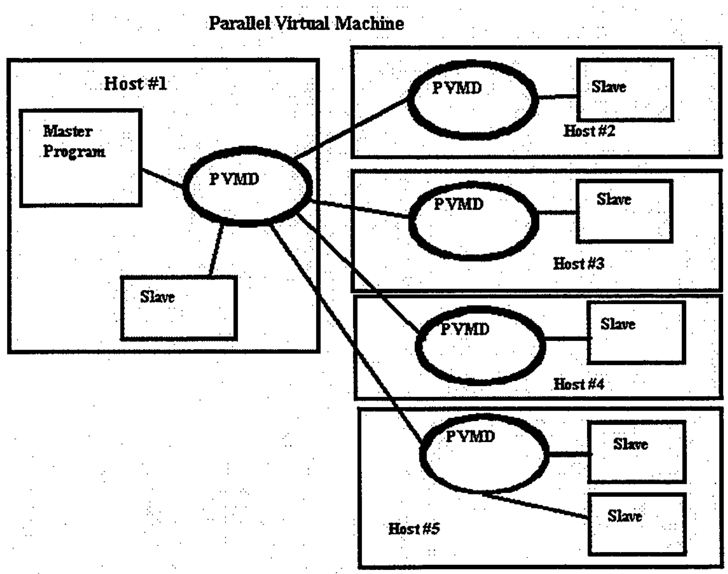

Figure 1. The master program sends and receives messages through the PVM daemon (PVMD) which routes the messages to other daemons on the way to and from slave modules. There may be multiple slaves on a single host and there is often both a slave and master program running on the same host.

Load Balancing

The key to success is balancing the computational load between machines /hosts /processors in the network. A heterogeneous network of workstations may contain a varied mix of slow and fast machines. Furthermore, as a computation proceeds, the load on each machine will change with time as users start-up and terminate other processes. Also, some machines may be on a local network and communications may be almost instantaneous while others may be further away on a wide area network and messages may require a greater time for delivery. Therefore, it is necessary to keep a concise database within the

master program of the relative performance of each processor. We use a very simple algorithm for load balancing. We keep a list of processors ranked by speed and we keep a list of tasks (frequencies) to be computed. We check off the tasks as they are completed and always send the next task to the fastest available host. Near the end of the computation, if we have sent each task out and we have available hosts we do not wait for slow hosts to complete their tasks but rather re-send those tasks out to the fastest available host. The goal is to keep all slave modules working. The resulting algorithm is therefore robust with respect to changes that do happen in the network(s) and on the various parts of the parallel virtual machine. The *master-slave* algorithm has been tested on a heterogeneous network consisting of 40 SUN, SGI, HP, and DEC workstations distributed over a corporate LAN and WAN. Floating point performance of the various workstations span nearly two orders of magnitude from a SUN SPARC-1 to a DEC 2100 5/250. The parallel virtual machine has been composed of machines at two locations in San Diego 10 miles apart connected by T1 and then bridged to machines located in Albuquerque connected on a leased line at 56KB.

The performance of each machine in the network reflects the time it takes to send and receive individual task messages as well as the speed and load of each machine. The net performance is almost always faster than the fastest machine in the network. Table 1 shows a compilation of runtime statistics for a test run on a very lop-sided mix of workstations. For each host we show the total number of frequency tasks completed, the average CPU time per task, the average latency time per task, and the relative speed rating. Each slave program reports the amount of CPU time that was expended in performing a task. Latency in this table is defined as the total time elapsed from the instant the master program sends a message to the slave program until the completion message is received by the master program minus the CPU time reported by the slave program. Latency is a practical measure that combines the communications time between master and slave with the amount of time the slave host was busy performing other tasks. The most responsive host, *decadent*, computed 154 of the frequencies using an average 0.634 CPU seconds/task plus an average latency time of 0.35 seconds/task during the coarse of the calculation. This mix of computers exhibited a range of over two orders of magnitude in relative performance. Several hosts contributed only 1 frequency task to the calculation due to a combination of slow machine and/or excessive CPU load on that host. The calculations were completed in about 65% of the time required to complete the calculations on the fastest machine alone. Obviously, a network of more evenly matched hosts will show more nearly linear speed-up as the number of independent hosts is added to the virtual machine.

Pseudo-Code For Load Balancing Data Base Structures

```
Task list (the "to do list")
        frequency, source location, receiver location,
        time started, time finished, slave processor
        finished/working/not-finished

List of slave processors (the "list of available workers")
        processor name and task id,
        total time on all tasks,
        number of tasks completed,
        average time per task,
        available/unavailable  (working/free),
        relative ranking by average speed
```

Figure 2. Pseudo-code for load balancing data structures.

Pseudo-Code For The Dynamic Load Balancing Algorithm

```
while ( frequency to do list not empty )
        check on incoming messages;
        if ( incoming message true ) then
        free processor in the list of available workers;
        update speed of processor in list of available workers;
        check off frequency on the frequency to do list;
        store results in the output file;
end if
if ( available processor true ) then
        get fastest processor from the list of available workers;
        get new frequency from the frequency to do list;
        send frequency task to processor;
end if
end while
```

Figure 3. Pseudo-code for load balancing. The goal is keep the fastest workers busy at all times until all tasks are finished.

Host	Number of Frequencies	Average CPU Time (sec)	Average Latency (sec)	Relative Speed
decadent	154	0.63463	0.35010	1000.00000
hoopy	54	2.60093	0.09255	244.00330
sundog	10	8.83578	7.33653	71.82554
sirius	8	18.77875	2.69360	33.79535
innelda	5	24.84400	2.52371	25.54478
indus	5	28.69200	3.53036	22.11887
incubus	5	37.55800	4.00099	16.89745
inxs	4	32.19750	4.33105	19.71068
insect	4	50.49750	4.70479	12.56764
inept	3	41.47333	6.93186	15.30223
intense	3	21.06000	27.92844	30.13459
infinity	3	60.39000	6.27558	10.50893
vulcan	3	54.64333	15.12743	11.61413
ingorant	2	32.02500	37.70395	19.81685
europa	2	46.80500	29.51931	13.55912
trantor	1	88.30000	23.33726	7.18725
austin	1	79.62000	40.04994	7.97079
coondog	1	96.35001	48.76627	6.58676
uranus	1	101.42000	45.21692	6.25749
terminus	1	100.68000	46.76197	6.30348
neptune	1	103.85999	53.99000	6.11048
total	271	-	-	-

Table 1. Runtime statistics for a typical calculation on a virtual machine consisting of 25 independent processors. Latency time combines communications time plus time a host is busy with other processes. Relative speed is based on the average total wall clock time required to complete a task which is the sum of the CPU and latency time.

The Wavenumber Integration Program

The resulting master and slave programs, ***prosem*** and ***proses***, are based on the wavenumber integration algorithm of Apsel and Luco (1983). A UNIX style manual page is included as an Appendix to this report. File formats and program options are discussed in the man page. The master program, ***prosem***, starts up the parallel virtual machine, spawns, the slave programs, ***proses***, on each host and saves the output frequency domain complex Green's function responses in a file. A second program, ***gseis***, is then run that computes the time domain Green's functions and stores them in *CSS 3.0* format with a *wfdisc* file (see Anderson et al. 1990a and 1990b for definitions of CSS 3.0 format). This seismogram format can be read and manipulated using a number of popular programs including the popular Seismic Analysis Code (SAC, 1995).

The Green's function responses for force components (Gzx, Gzz, Gxz, Gxx, Gyy) and moment tensor components (Gzzz, Gzxx, Gzxz, Gzyy, Gxzz, Gxxx, Gxxz, Gxyy, Gyxy, Gyyz) are each provided as well as special purpose sources such as an isotropic moment tensor (explosion/implosion) (Gzi, Gxi), a horizontal tension crack (Gztc, Gxtc), and a vertically oriented compensated linear vector dipole (Gzclvd, Gxclvd). The special moment tensor sources are defined as; isotropic: Mxx = Myy = Mzz, horizontal tension crack: Mxx = Myy = Mzz (m/(l+2m)), and vertical CLVD; Mxx = Myy = - Mzz / 2. The right-hand coordinate system is defined where X is radial from source to receiver and Z is up. All Green's functions are the velocity response (meters/second) for a step function source (either Newtons for force components or Newtons-meters for moment tensor components). Therefore as examples, Gzz is the vertical velocity response for a step function vertical force, Gyy is the transverse velocity response for a transverse step function force, and Gzxz is the vertical velocity response for the XZ source couple, Mxz.

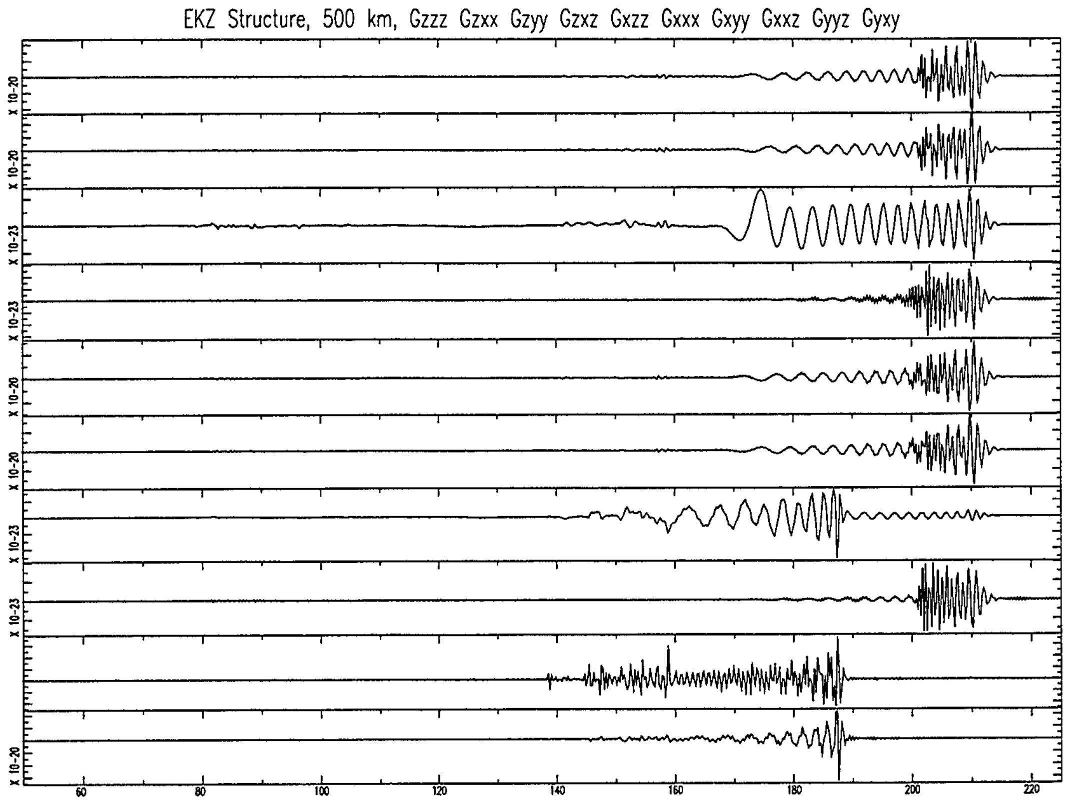

Figure 4a. Example of moment tensor component Green's functions, Gzzz, Gzxx, Gzyy, Gzxz, Gxzz, Gxxx, Gxyy, Gxxz, Gyyz, Gyxy, for an East Kazakhstan Structure.

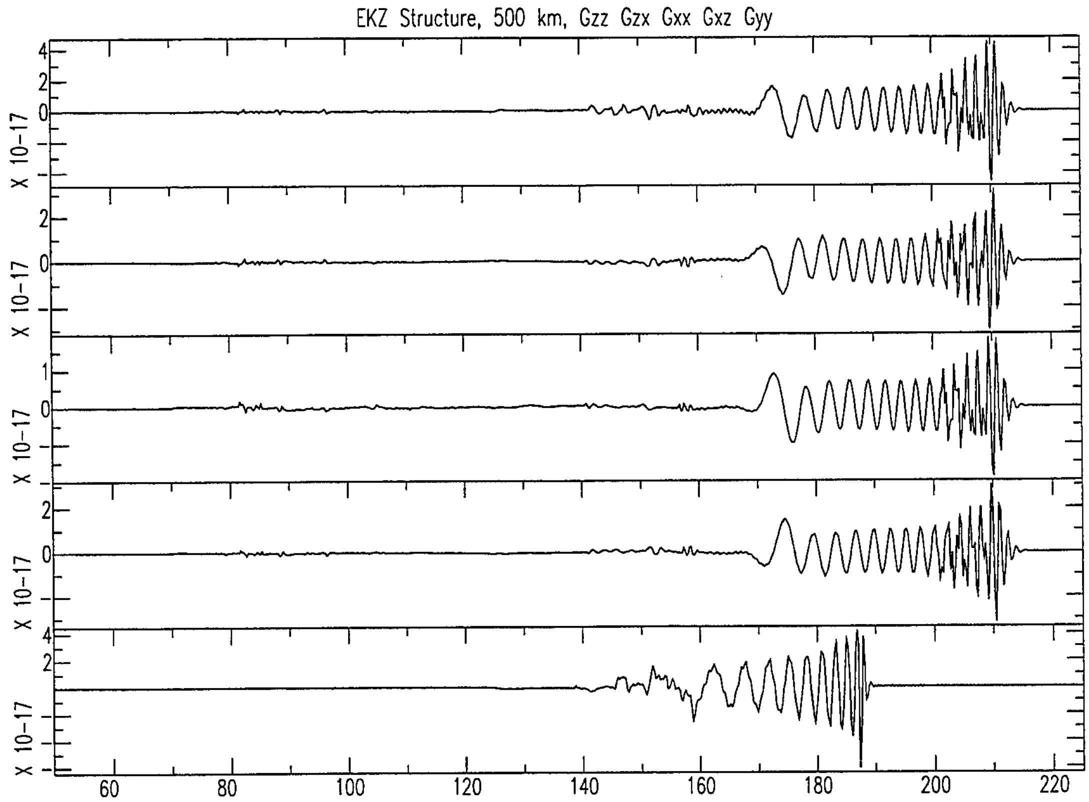

Figure 4b. Example of individual force component Green's functions, Gzz, Gzx, Gxx, Gxz, Gyy, for an East Kazakhstan Structure.

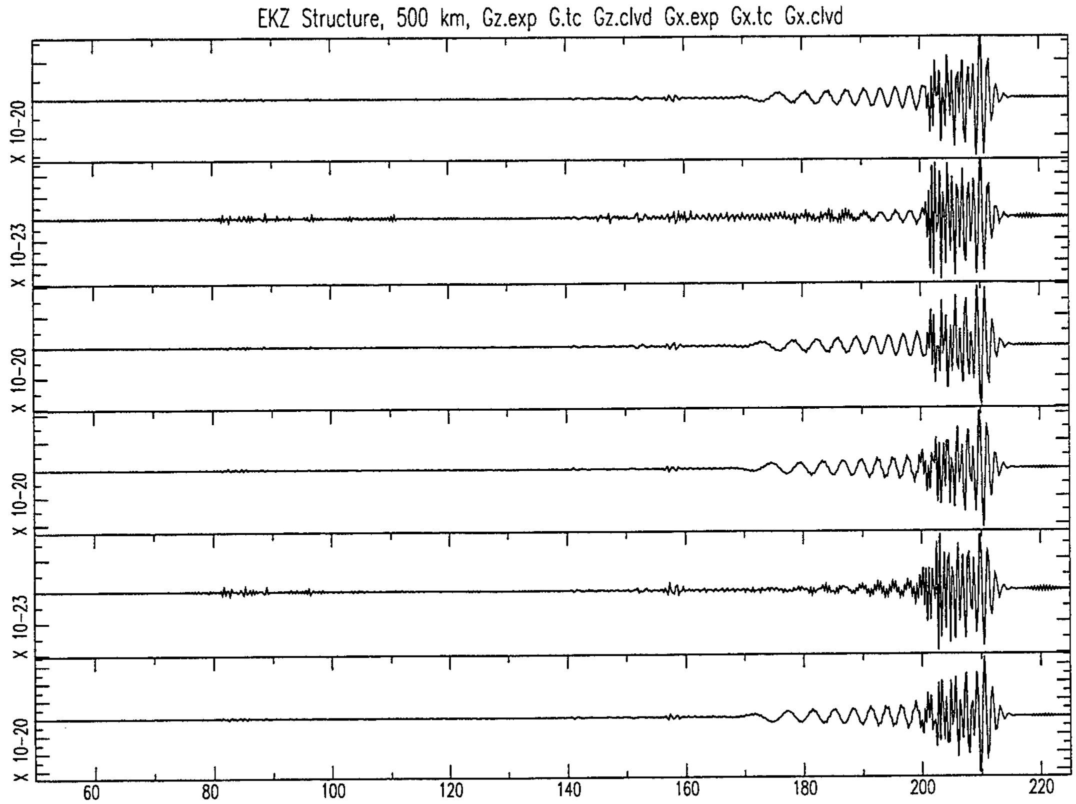

Figure 4c. Example of special source Green's functions, Gzi, Gztc, Gzclvd, Gxi, Gztc, Gxclvd, for an East Kazakhstan structure.

Research Progress

A beta test version PVM based parallel wavenumber integration program has been developed that computes Green's functions in CSS 3.0 format readable with SAC. Near linear speed-up over single processor has been realized with a heterogeneous network of SUN OS4/Solaris, HP, SGI, and DEC workstations tested over WAN and LAN. The software requires PVM 3.3.11, a FORTRAN F77 compiler, and a C compiler. The Gnu-*make* program is recommended on SGI, HP, and DEC workstations. Interested beta testers should contact Keith L. McLaughlin (*scatter@maxwell.com*). Current information on the availability of the software can be found on the Internet at *http://www.maxwell.com/products/geop*.

Future Plans

Changes will be made to the PVM based parallel wavenumber integration program to fix bugs that surface under beta testing. Frequency dependent attenuation, Q(f), will be added to the layered earth model. An X-windows graphical user interface to the wavenumber integration program that is in alpha testing will be released for beta testing.

Tests have begun to examine limitations of using layered Earth structures (1D models) to model principal features of regional seismograms in the presence of lateral heterogeneity. 3D finite difference calculations have been performed with lateral heterogeneity superimposed upon a layered structure. Additional calculations will be performed in the next few months. Layered earth model synthetics will be used to compare an ensemble of seismograms from randomly layered 1D models with synthetic seismograms from realistic 3D heterogeneity.

A library of synthetic seismograms is to be assembled based on a wide variety of crustal models. The surveys of Christensen and Mooney (1995) and Mooney, *et al.* (1996) will serve as the basis for a library of rough crustal models. Random layering as suggested by the comparison of 1D and 3D modeling will be inserted into the models.

Acknowledgments

We wish to thank Al Geist and Bob Manchek of ORNL and UT for an excellent PVM tutorial at Supercomputing '95. Steve Day of SDSU provided many useful suggestions in the implementation of the wavenumber integration code.

This work was sponsored by the U.S. Department of Energy Office of Nonproliferation and National Security issued by the Phillips Laboratory under contract no. F19628-95-C-0207.

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Appendix - Manual Page for Prosepvm

NAME

prosepvm - synthetic seismograms by wavenumber integration

SYNOPSIS

prosem [pvm/nopvm] [nohalt]
proses

DESCRIPTION

Prosepvm calculates complex spectral linear elastic responses for point forces in general layered structures. These responses may be used to form Green's functions for synthesis of seismograms from seismic source representations such as forces or moment tensors.

Prosepvm uses a portable message-passing programming system (PVM), designed to link separate host machines to form a "virtual machine." It works in master/slaves mode with com- munication between master and slaves only (no communication between slaves). Program has an argument (pvm or nopvm character flag). Default is no flag (pvm case) In case of nopvm the program runs on a single machine.

The program consists of two executables: prosem is master program and proses is slave program. User has to take several steps to be able to execute the program:

1. Define in your home/.cshrc file
   setenv PVM_ROOT .../pvm3
   setenv PVM_ARCH SUN4
   setenv PVM_LIB $PVM_ROOT/lib
   source .cshrc
   Each computer must have these environment variables set in the .cshrc file.

2. Each computer must have pvm3.3.11 software in pvm3 directory and proses has to be compiled on this machine using PVM.

3. Copy proses to slaves to the default location $PVM_ROOT/bin/PVM_ARCH for each computer in the network.

4. cd to your working directory

5. Prepare hostfile (file containing list of all machines). See below for sample hostfile. some output files and produce the synthetic seismogram files.

6b. Or execute prosem[nopvm] < Input_file

Prosem has at most 2 arguments: First argument is pvm (PVM) or nopvm (NOPVM). If none pvm or nopvm appears, it means pvm run. Second argument is halt(HALT) or nohalt(NOHALT) to halt all processors in hostfile.

FILES

Earth model file is in a standard S-CUBED format where nly is number of layers, iunits = 0 MKS units, iunits = 1 for Geophysical units. If MKS UNITS then displacement output is in meters, velocity in meters/sec, density in kg/m^3, stress in Pascals (Nt/m^2). Geophysical (iunits=1) (inputs are in g/cm^3, km/sec, km) units. If Geophysical units are used, they are converted to MKS.

Layers of model are specified as

th(i),alpha(i),beta(i),rho(i),qm(i),qk(i),i=1...nly

where th() layer thickness, alpha() p wave velocity, beta() s wave velocity, rho() density, qm(), shear modulus Q and qk() bulk Q, respectively, beginning at the surface layer (i=1).

The namelist file contains values for control variables; namelist /iprose/ prnt,displ,stress,fluid,nr,nz,nzs,ri,dr,zi,dz,zsi,dzs,r,z,zs,srctyp,rngord, cylind,nrng,rngrad, nfreq,fi,df,errlm,sdkmn,nkmx,reflay,usevel,sklim

* Diagnostic printout flags:

  Prnt(i) (logical) i=1...6 controls printout level where prnt(1) = t prints namelist control, prnt(2) = t prints model heading, prnt(3) = t prints 2 line summary for each frequency, prnt(4) = t prints all integrals for each frequency, prnt(5) = t prints summary of each k integration step, prnt(6) = t prints additional details of each int step. Default values are prnt(1-3)=.true., prnt(4-6)=.false.

* Output control flags:

  Displ (logical) = t output displacements.

  Stress (logical) = t output stresses.

  Fluid (logical) = t for fluid layer at surface (default=false).

Reflay (integer) reference layer used to form dimen- sionless quantities (default= 1).

Usevel (logical) = t (default=true) to keep the effec- tive shear and compressional wave velocities the same as inputed. If false the effective velocities will be increased by factors of sqrt(1.+(1./q(i))**2), where q(i) represents the Qbeta and Qalpha for layer i.

* Source-Receiver geometry:

nzs (integer) number of source depths zs(i) i=1...nzs source depths in order of increasing depth. or zsi,dzs initial and incremental source depth: zs(i)=zsi+(i-1)*dzs if dzs greater than 0.

nz number of receiver depths.

z(i) i=1...nz receiver depths in order of increasing depth. or zi,dz initial and incremental depth: z(i)=zi+(i-1)*dz if dz greater than 0.

nr number of epicentral distances

r(i) i=1...nr receiver ranges in any order or ri,dr initial and incremental ranges: r(i)=ri+(i-1)*dr if dr greater than 0.

srctyp (integer) defines source type: = 0 for point force = 1 for point explosion

* Frequency range specifications:

nfreq number of frequencies to compute

fi, df initial and incremental frequencies. if df .gt. 0. the next fi is given by fi+df.

dfgrow used with fi and df only if df .lt. 0. so that next fi is given by dfgrow*fi - df.

or frq(i) i=1...nfreq actual frequencies used only if df.eq.0 and nfreq must be .le. 50 to use this option.

* K integration definitions:

nklim number of k intervals to integrate over (default: 1).

klim(i) i=1...nklim+1 defines the k intervals. The j-th interval extends from klim(j) to klim(j+1). If nklim=1 then the upper limit of integration is set by prose between klim(2) and klim(3). Default: klim = 0., 1.5, 1.e20.

dkmn minimum allowable k increment (default: .0001).

nkmx maximum number of k steps allowable (default: 2500).

ndig number of significant digits required from integration procedure (default=3). Note: still must set the variable errlm for sampling criterion (which depends on the computer as well as the type of run).

errlm controls the accuracy of the numerical integra- tion. errlm=.1e-5 normally gives 5 significant figures

ASCII output file contains misc. output from the run.

Binary header output file contains important variables needed to interpret the binary spectral output.

Binary spectra output file contains the complex spectra of the fundamental responses. Output (for each frequency) displacements and stresses are found in the array rsp for all epicentral distances and receiver depths due to all the sources.

If srctyp=0, the 15 components due to each point force are arranged as follows;

displacements: i=1,2 are for vert. point force: ur,uz i=3,4,5 are for horiz. point force: ur,uphi,uz stresses: i=6,7,8,9 are for vert. point force: sigmarz, sigmazz, sigmarr, sigmaphiphi, i=10, 11, 12, 13, 14, 15 are for horiz. point force: sigmarz, sigmaphiz, sig- mazz, sigmarr, sigmaphiphi, sigmarphi.

If srctyp=1, the 6 components due to each point explosion are arranged as follows;

displacements: i=1,2 ur,uz stresses: i=3,4,5,6 sigmarz,sigmazz,sigmarr,sigmaphiphi

The displacements and stresses have units of force. To get real dimensional quantities, the displacements should be divided by a factor of (shear mod. of reference layer times r) where shear modulus = (rho1*beta1**2) with rho1=rho(reflay), and beta1=beta(reflay) (reflay=1 by default), and the stresses should be divided by a factor of (r**2). These quantities may be found in binary header file.

Note that to get results in the time domain, these frequency domain results have to be be transformed into time for a given r,z,zs using an FFT algorithm. The results have to be multiplied by a factor of (2.0*pi*df) in which df is the increment of the frequency points in hertz, so that (1./df) is the amount of total time signal.

For results to a double couple source function, reciprocity is employed so that the results at the receiver are found by calculating the stresses at the depth of the double

couple. Then a rotation of the stress tensor is performed to achieve the desired orientation of the double couple.

SEE ALSO

gseis(1) for conversion of binary spectral output to synthetic seismograms.

AUTHOR

Original code by R. Apsel, many modifications by Boris Shkoller and K. L. McLaughlin (S-CUBED) to convert to UNIX environment and modify i/o.

SAMPLES

```
#Example 1. Hostfile is used just for illustration
vulcan
sirius
# multi=decadent,2;
decadent
tequila
neptune
pluto
europa
camel
eeg
renoir
trantor
titan
earth
austin
coondog
oberon
terminus
uranus
Sun4c.scubed.com
shark
```

Example 2. Namelist is used just for illustration

```
$iprose
prnt=t,t,t,t,f,f,
displ = t,stress = f ,fluid = f,
nr= 1 , nz = 1, nzs = 1,
ri = 1000.0 , dr= .0,
zi = 0.0 , dz = 1000.0,
```

```
    zsi = 680.0 , dzs = 1000.0,
    r = 100000.,
    srctyp = 0,
    nfreq = 257 , fi = 0.0 , df = .0078125,
    errlm = 1.e-6 ,sdkmn = e-6,
    nkmx = 99000 , reflay = 1,
    usevel = t,
    sklim = 0.0 , 1.5 , 1.e20 ,
$end
```

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